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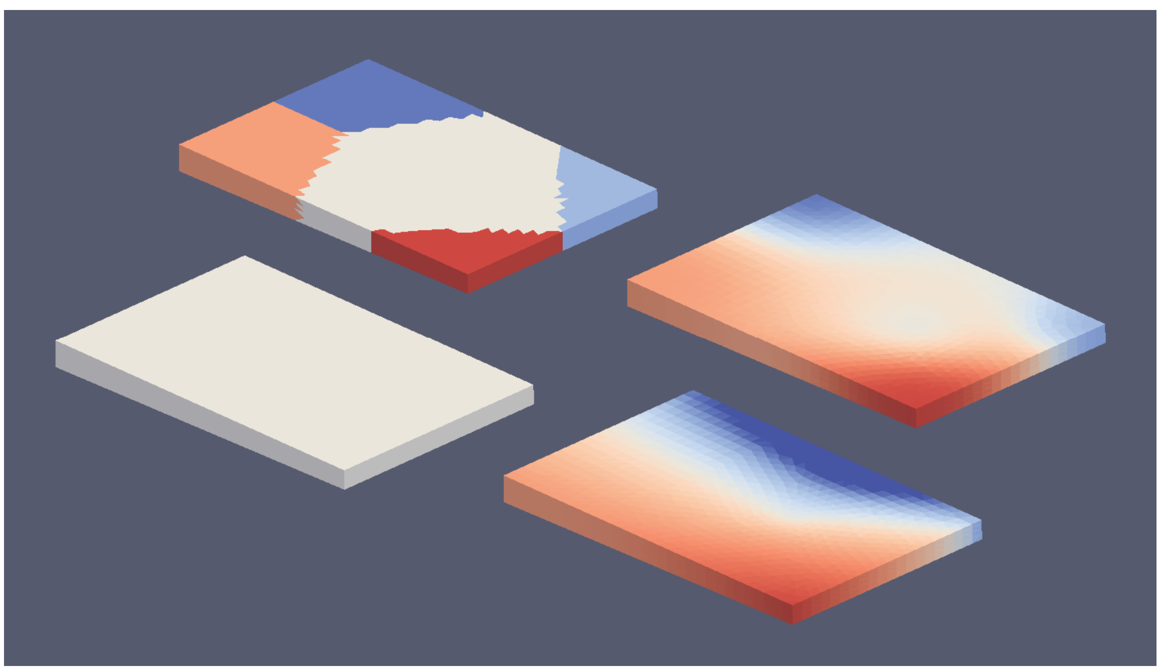
# Adaptive Hydraulics/Hydrology (AdH) Pilot Point Specification

## Guidelines for Solving 3D Groundwater Problems Utilizing Pilot Points

Kevin D. Winters

November 2013



# Adaptive Hydraulics/Hydrology (AdH) Pilot Point Specification

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# Abstract

Guidelines are presented herein for using the US Army Corps of Engineers (USACE) Adaptive Hydraulics/Hydrology (AdH) modeling software to model three-dimensional groundwater problems with constituent or heat transport utilizing pilot point specification. Pilot point specification is an auxiliary module intended to be a flexible method to specify spatially-varying parameters that supersede the traditional uniform parameters in the model. Examples of such parameters are hydraulic conductivity, porosity, and mesh refinement. Spatial variation can be used to develop high-fidelity computer models. This document contains descriptions of the pilot point input cards and examples.

The pilot point specification module is currently integrated into the AdH Groundwater code (kernel version), but can be extended to additional AdH physics modules as necessary. Input is currently manually generated with result viewable utilizing the open-source ParaView visualization software.

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# Preface

This report is a deliverable product under the military direct-alloted Department of the Army Project AT 40, Work Package AT 40-512, Geoenvironmental Tactical Sensor Simulation (GEOTACS) Work Unit AT40GT-036, CTB System Processes and Analyses, and was part of an Army Technology Objective.

This report was prepared by Kevin D. Winters, Hydrologic Systems Branch (HFH), Flood and Storm Protection Division (HF), Coastal and Hydraulics Laboratory (CHL), US Army Engineer Research and Development Center (ERDC), Vicksburg, MS, under the general supervision of Dr. Aaron R. Byrd, P.E., Chief, HFH; Dr. Ty V. Wamsley, Chief, HF; and José E. Sánchez, P.E., Acting Director, CHL. Supervision was provided by Stacy E. Howington, Principle Investigator, GEOTACS, and Joshua Fairley, Work Package Manager, GEOTACS.

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Contributors to this work include Stacy E. Howington, Amanda M. Hines, Clarissa M. Murray, and Ryan E. Pickett.

# Unit Conversion Factors

| Multiply | By | To Obtain |
|---|---|---|
| fathoms | 1.8288 | meters |
| feet | 0.3048 | meters |
| inches | 0.0254 | meters |
| microns | 1.0 E-06 | meters |
| miles (nautical) | 1,852 | meters |
| miles (US statute) | 1,609.347 | meters |
| yards | 0.9144 | meters |

# 1 Introduction

Often, a groundwater model starts with the process of simplifying geologic data (e.g., bore logs) into hydrogeologic units to create a conceptual geologic model. Each unit is a zone of similar soil characteristics that affect groundwater flow. This zonal classification or zonation process generalizes a complex system into regions of homogeneous soil, limiting heterogeneity to differences between hydrogeologic units. To include realistic heterogeneity in the geologic model, many zones with the proper spatial distribution may be necessary. Each additional zone may represent the same basic soil type but with slightly different characteristics. Once a conceptual geologic model is finalized, it informs the creation of the computational domain with a partition or region for each zone. Each domain partition is assigned a set of material properties endowing the domain with material regions, each with uniform characteristics.

The inclusion of spatially varying material properties with smooth transitions is not practical with zonal classification. To overcome this limitation, the finite-element software framework AdH (Berger and Howington 2002; Pettway et al. 2010) now allows specific material properties to vary smoothly through the domain with the use of pilot points. The material region, or more specifically, the partition assigned the material property, acts as the ultimate extent of the variation. In this way, pilot point specification complements zonal classification by permitting heterogeneity to be defined within a partition.

Pilot point specification consists of one or more groups of the following three components:

- set of spatial coordinates with values
- interpolation method
- parameter association.

A pilot point is a coordinate location with a given value or values. A collection of pilot points includes enough information to sufficiently describe a parameter distribution field in space to approximate an unknown physical parameter. Given an interpolation method, the provided point data will create a spatial distribution of the unknown

physical parameter on the computational domain. Once associated with a material property, the pilot point group replaces the standard uniform value of the material property; a value is now specified at the level of an individual element rather than the material region. Each pilot point group describes a unique parameter distribution field, such as the variability of hydraulic conductivity in a soil.

While pilot point specification could completely replace zonal classification, by declaring the entire domain as a single partition and describing soil properties that range across major soil types, this is, in general, not advisable. Not all material properties are compatible with pilot point specification such that completely different soils are not possible. For example, water retention curves cannot be representative of both sand and clay soils. It is better to use standard zonal classification to describe major heterogeneity (between soil types) and pilot point specification for minor heterogeneity (internal to a soil type).

The original concept of pilot point specification focused on the spatial variation of basic soil characteristics. The method's usefulness has been extended to include most material properties, mesh adaption control, and initial conditions.

The following sections provide a brief example of pilot points incorporated in a simulation (Section 2) and discussions of pilot point methods implemented by AdH, input control cards, output data (Section 3), and AdH model execution (Section 4).

# 2 Example Simulation

A fictional *box* simulation is presented here to showcase aspects of pilot point specification. The intent of this example is to contrast the results of a base simulation (standard AdH input) and simulations utilizing pilot points. Familiarity with the AdH model is assumed (documentation and examples available at http://adh.usace.army.mil/). A detailed discussion of pilot point methods and specification is provided in Section 3.

## 2.1 Base Simulation

The domain is a 90-m by 60-m rectangular prism with a flat, inclined surface sloping from a height of 15 m to 12 m at the opposite longitudinal edge as shown in Figure 1. The domain includes three partitions, representing a silt soil (Material 1) overlying a clay soil (Material 2), overlying a sand soil (Material 3). A flow field was induced by specifying head values of 13.5 m and 11 m on the opposing longitudinal vertical faces. These boundary conditions are hydrostatic with all remaining faces assigned no-flow boundary conditions. An extraction well that is screened in the bottom hydrogeologic unit, Material 3, was located two-thirds down the longitudinal ($x$-axis) centerline. The simulation was defined using the standard AdH input cards for groundwater problems, including zonal hydraulic conductivities, and run to an equilibrium state (Figure 1). Material 2 acts as an aquitard suppressing the effects of the extraction well from Material 1 (the effects cannot be seen in Figure 1). Material 3 is the preferential pathway for flow since the sand is most permeable.

## 2.2 Inclusion of Pilot Points

Next, pilot point specifications were included to depict the variation of hydraulic conductivities in each hydrogeologic unit. For convenience, hydraulic conductivity scaling values instead of hydraulic conductivity parameter values are given at each domain corner and the well for each material type (Section 3 details the available options for specifying hydraulic conductivity). The resulting hydraulic conductivity values at the domain corners are listed in Table 1. Cardinal directions are used to denote the domain corners with the positive $y$-axis direction aligned with North. It is noted that the pilot points located at the well have scalar values of 1.0 that reproduce the zonal hydraulic conductivity values used in the base

Figure 1. Example computational domain showing zonal hydraulic conductivities ($K_H$ ) and pilot point locations as yellow cylinders (A), and the computed total head solution (B).

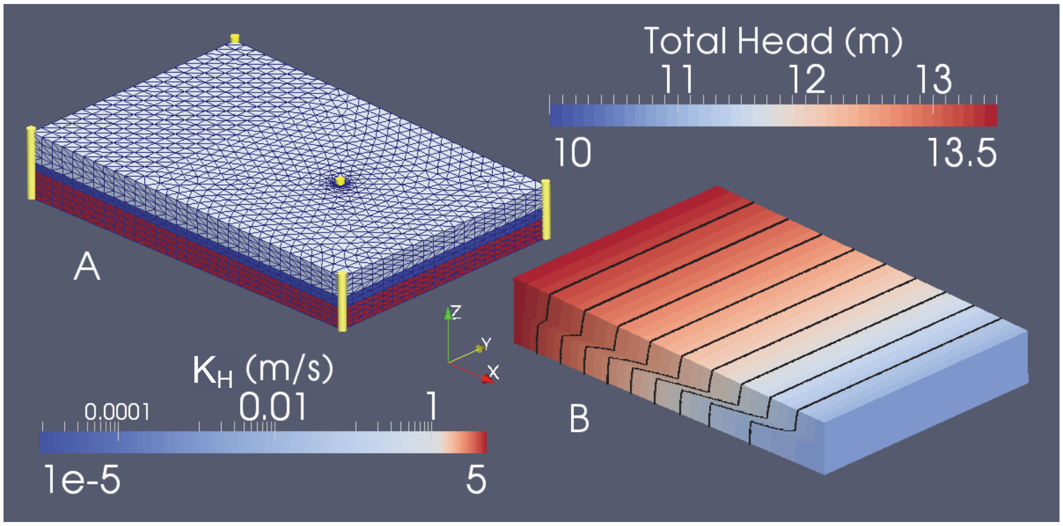



Table 1. Specified Hydraulic Conductivities for Example Simulation

| | Horizontal Hydraulic Conductivities, $K_H$ (m/day) | | | | | |
|---|---|---|---|---|---|---|
| | | Pilot Points | | | | |
| Material | Zonal | NW | NE | SE | SW | Well |
| 1 (silt) | 0.300 | 0.0660 | 0.276 | 1.01 | 0.645 | 0.300 |
| 2 (clay) | 1.00e-5 | 5.40e-6 | 2.27e-5 | 1.60e-6 | 5.32e-5 | 1.00e-5 |
| 3 (sand) | 5.00 | 0.81 | 1.74 | 37.7 | 15.9 | 5.00 |

simulation. The five point locations are depicted in Figure 1. Each material type has a pilot point group associated with the hydraulic conductivity tensor. The scaling values are interpolated to the elements assigned the respective material type and alter the hydraulic conductivity tensor used in the system of groundwater equations. The solution will then be based on values specific to each element as well as the non-varying material properties.

The *box* simulation was run with each available interpolation method (natural neighbor, inverse-distance weighted, and ordinary kriging; described in Section 3) using the same pilot point values. The resulting hydraulic conductivity fields generated by pilot point specification are displayed in Figures 2 through 4, contrasted by the original base simulation zonal values. Pilot point specification created asymmetrical, macroscopic effective conductivity zones across each material layer (hydraulic conductivity is still isotropic locally). Figures 5 and 6 show the resulting head

Figure 2. Comparison of the horizontal hydraulic conductivity ($K_H$) of Material 1 using a variety of methods: (A) zonal, (B) nearest-neighbor, (C) inverse-distance weighted, and (D) ordinary kriging.

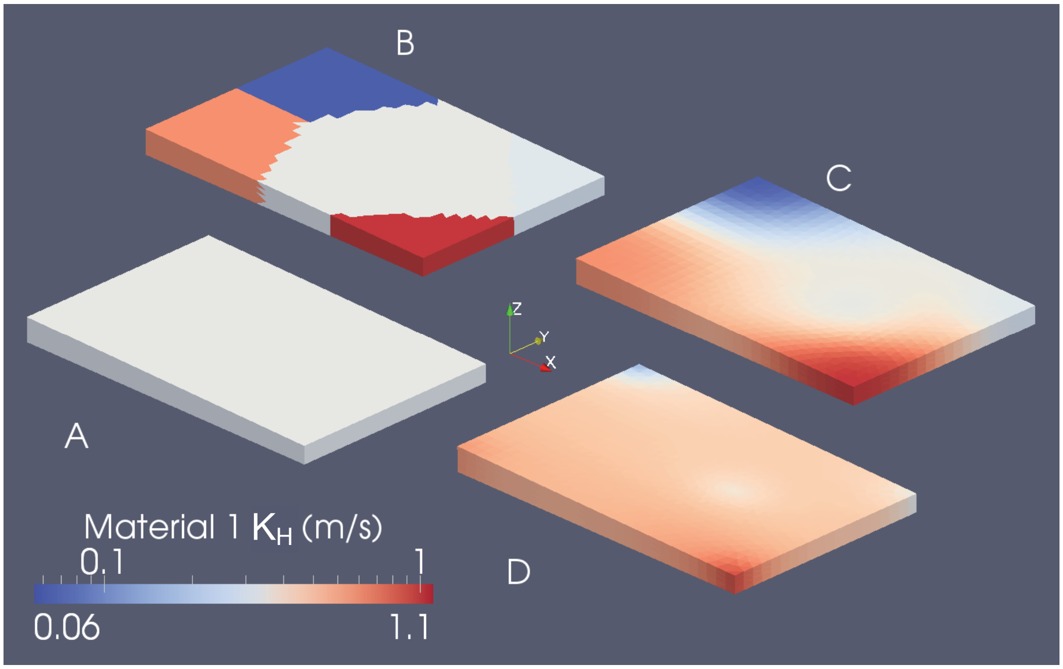



Figure 3. Comparison of the horizontal hydraulic conductivity ($K_H$) of Material 2 using a variety of methods: (A) zonal, (B) nearest-neighbor, (C) inverse-distance weighted, and (D) ordinary kriging.

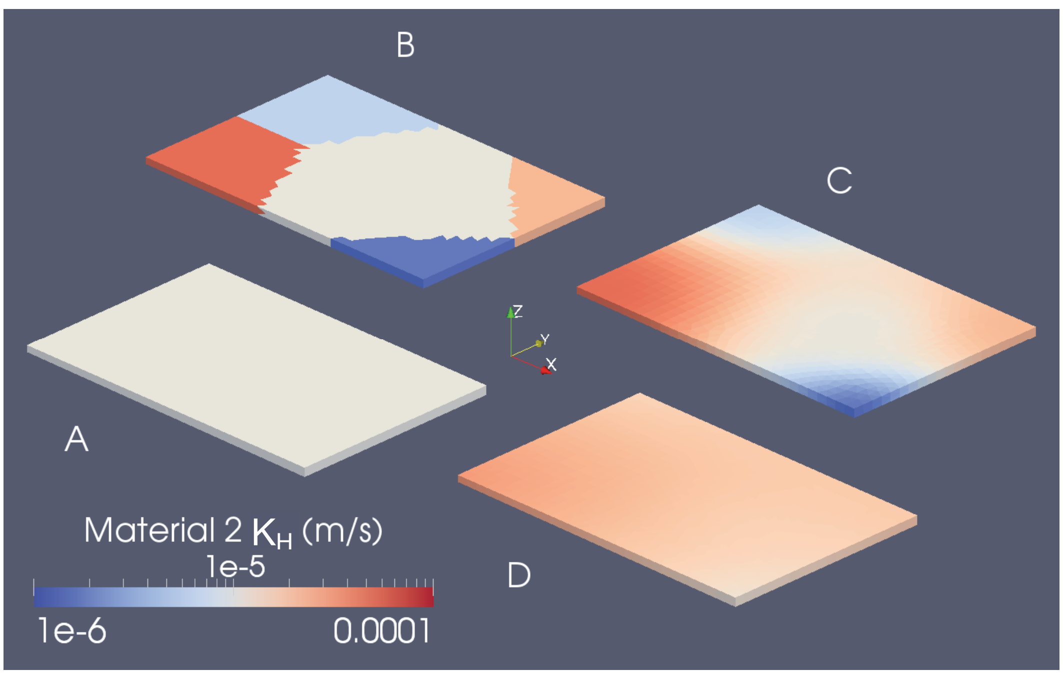


Figure 4. Comparison of the horizontal hydraulic conductivity ($K_H$) of Material 3 using a variety of methods: (A) zonal, (B) nearest-neighbor, (C) inverse-distance weighted, and (D) ordinary kriging.

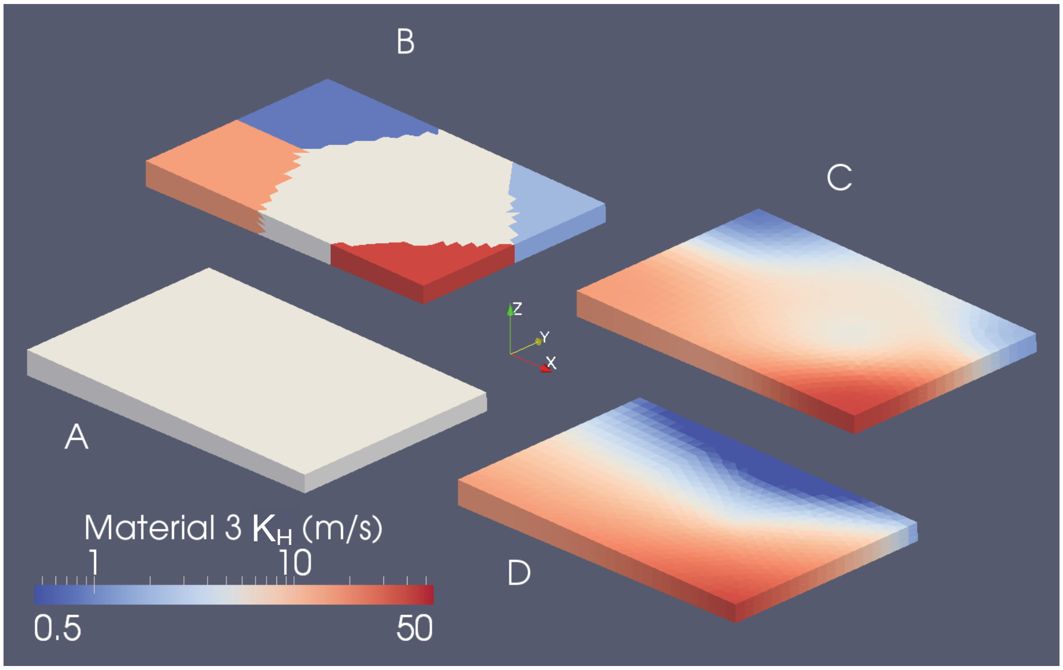



Figure 5. Comparison of the total head solution based on a variety of methods to describe hydraulic conductivity: (A) zonal, (B) nearest-neighbor, (C) inverse-distance weighted, and (D) ordinary kriging.

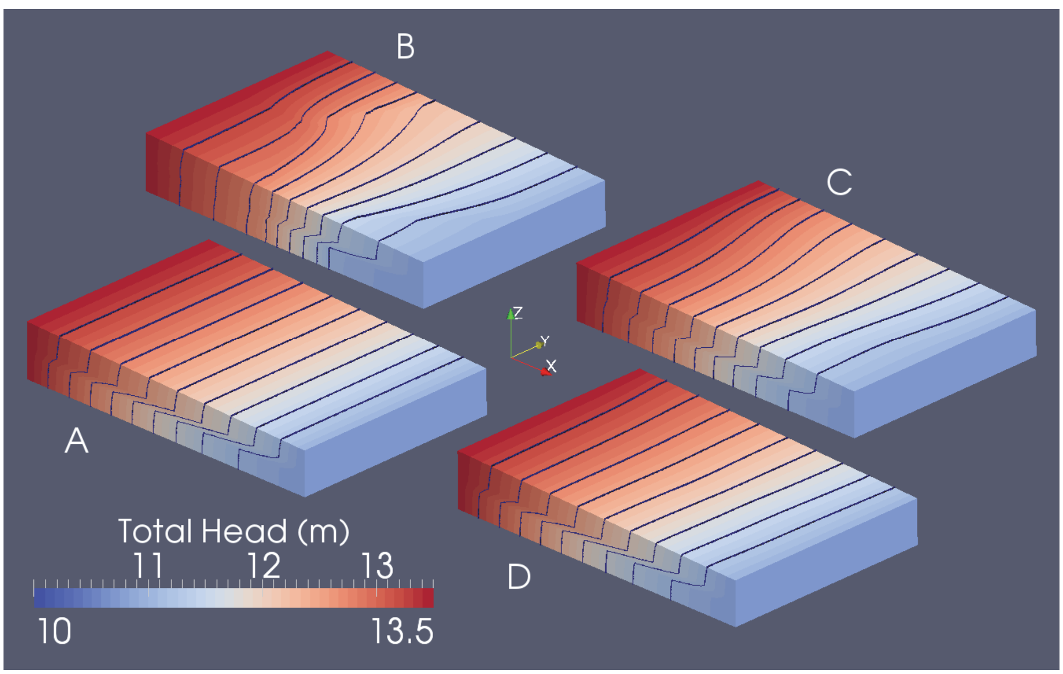
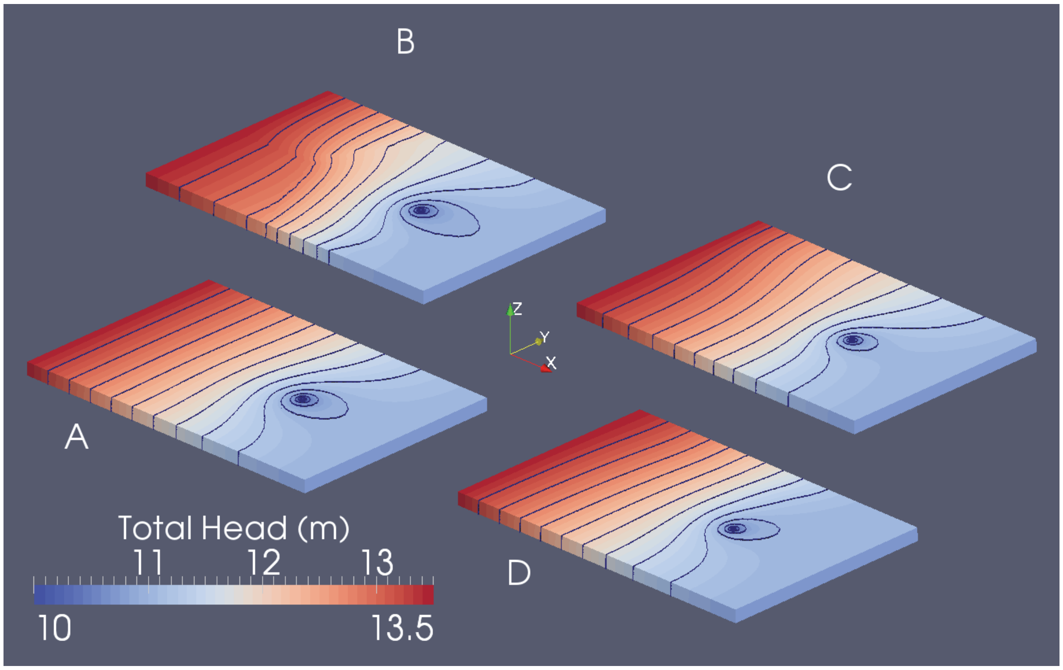


Figure 6. Comparison of the total head solution, clipped through Material 3 to show influence of extraction well, based on a variety of methods to describe hydraulic conductivity: (A) zonal, (B) nearest-neighbor, (C) inverse-distance weighted, and (D) ordinary kriging.




solutions of the full domain and the domain clipped at 3.5 m to highlight the influence of the extraction well, respectively. Looking specifically at the lowest hydrogeologic unit, Material 3, the permutations generated zones of higher and lower permeability generally parallel to the macroscopic flow field (longitudinal axis). The connectivity of the similar zones and the smoothness of variations are dependent on the interpolation method employed. These hydraulic conductivity zones bend the head contours from the original symmetrical solution producing differing well-capture areas in the confined aquifer.

## 2.3 Review

While this example shows the successful inclusion of a spatially varying material property, it is also provided as a cautionary tale. It is easy to append a standard AdH simulation with pilot point specification and generate complex soil characteristics, but it may not be beneficial. The domain is split by an aquitard such that the hydraulic conductivity of the layers may be inconsequential beyond their relative magnitudes depending on the purpose of the model. For example, if the intent is to verify the extents of the capture zone of the extraction well, then pilot points only for Material 3 could be added after verifying that it is indeed within a confined aquifer. On the other hand, pilot points could be added only for Material 1

when determining the location of the water table. Additionally, the permeability of the clay, Material 2, is almost small enough to be considered a solid, computationally. Though this problem size is small, each pilot point parameter taxes the model resources by requiring additional memory allocation, computations, and logical operations. These effects are scaled as the problem size increases. Finally, it is important to utilize the appropriate interpolation method to describe significant spatial variation of the distribution field.

Ideally, pilot point specification for material properties would be used in conjunction with parameter estimation methods to calibrate results with observed data. New parameter values can be iteratively replaced in the pilot point specification without the need to edit the original AdH input definition of a soil. Thus, pilot points serve to regularize an otherwise difficult parameter estimation problem. Pilot point specification should be included only after the groundwater system is well understood, the regular zonal classified simulation is run, and the results indicate specific areas of the domain that need to be addressed further.

# 3 Methods and Files

To assist the user, this section combines two essential discussions of pilot point specification, the implementation of methods within AdH and the input and output files. The desire is to ensure clarity when seeking information of a given pilot point card. File cards are bolded in the document body for ease of use.

## 3.1 Input

Since pilot point specifications supersede the standard input, the location of the pilot point cards was designed to be flexible. The default location to provide pilot point cards is a new ASCII text file given the simulation base name with the designation “pp” as the extension. For example, if the AdH simulation is named “my_sim” (i.e., my_sim.bc) then the default location is the file my_sim.pp. Alternatively, the pilot point cards may be provided in files otherwise named if referenced within the AdH super file (*.sup) with the **PP** card (Example B and Example C in the Appendix). This flexibility permits the specification of pilot points within the standard AdH input file (*.bc) or across multiple files. See the appendix for examples of input file combinations.

Currently, the pilot point input must be manually generated; a complete graphical user interface (GUI) to generate the input will eventually be available in the Computational Model Builder (CMB, developed by Kitware, Inc., for ERDC) suite’s ModelBuilder tool. Specified pilot point information supersedes original information only if the operational parameter card **OP PP** is inserted in the input file; otherwise, provided pilot point information is ignored, and the original information retains its precedence.

The pilot point specification cards, listed in Table 2 and described in the following subsections, may appear in any order with the cards forming sets linked together by unique pilot point group IDs. Pilot point specification utilizes IDs that are *not* restricted to the one-based, sequential limitations of other AdH IDs; IDs may be positive or negative and are limited only by the operating system’s definition of an integer. It is best practice to choose predetermined ranges of IDs to represent parameters for easy inclusion into the simulation. For example, single or double digit IDs could represent specific initial conditions while larger numbers could refer to specific

materials by incorporating the material ID (25010 and 25020 could allude to material 25). In this way, different combinations of pilot point specification can be included without renumbering the input.

Table 2. Control Card Categories

| Card | Description |
|---|---|
| **Operation Parameters** | (**Section 3.1.1** and **Table 3**) |
| OP PP | Enable Pilot Point Specification |
| **Pilot Point Specification** | (**Section 3.1.2**) |
| **Association Parameters** | (**Section 3.1.2.1** and **Table 4**) |
| PP HOT | Initial Condition Parameter |
| PP MP | Material Parameter |
| **Group Properties** | (**Section 3.1.2.2** and **Table 5**) |
| PP LIM | Interpolation Limits |
| PP PT2 | 2D Pilot Points |
| PP PT3 | 3D Pilot Points |
| PP RAD | Search Radius |
| PP TYP | Interpolation Method |
| **Kriging Interpolation Properties** | (**Section 3.1.2.3** and **Table 6**) |
| PP KRG | Kriging Information |
| PP VGC | Variogram Contributions |
| PP VGI | Variogram IDs |
| PP VGS | Variogram Sill |
| PP VGW | Variogram Weights |
| PP VG2 | 2D Variogram Information |
| PP VG3 | 3D Variogram Information |
| **Miscellaneous** | (**Section 3.1.2.4** and **Table 7**) |
| PP DBG | Debug Information |

Table entries are hyperlinked.

Comments are permitted in the input files if demarcated with a preceding *#* or *!*; all text after the delimiter on the file line is ignored. Blank lines are also permitted. The AdH pilot point file input routines will validate the cards and provide information and error messages to assist correct card

specification. AdH will exit after listing any errors and before pilot point interpolation and normal simulation operation occurs.

### 3.1.1 Operation Parameters

The problem type and operational methods of AdH are controlled by the operational parameter cards, which are denoted by **OP** card type. To utilize the pilot point specification in a groundwater and/or heat transport model, the **OP PP** card (Table 3) must be included with the normal operational parameter cards. This card is the flag for AdH to perform the auxiliary logical operations to support pilot points. AdH performs the standard model operation, specified by the normal operation parameters (e.g., **OP GW**) if pilot point cards (**PP** card type) are given and **OP PP** card is excluded.

Table 3. Operation Parameter Cards

| OP PP | ENABLE PILOT POINT SPECIFICATION | | |
|---|---|---|---|
| The OP PP card enables the operation of pilot point specification and must be included only in the standard AdH input file (*.bc). | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | OP | Card type |
| 2 | string | PP | Parameter |

### 3.1.2 Pilot Point Specification

Pilot point specification cards are identified by the designation **PP** and are sorted into subcategories described in the following subsections. There will be a set of cards for each pilot point group included in the model.

#### *3.1.2.1 Association Parameters*

These cards specify the spatially varying simulation parameter that a pilot point group represents. A pilot point group may only be associated with a single parameter: an initial condition or a material property.

Pilot point groups may describe any of the available initial condition types for groundwater (pressure head or total head and concentration) and heat transport problems (temperature) by the **PP HOT** card. The specification is applied to the entire domain by interpolating values at all node locations. The standard hot file is still required by AdH; therefore, pilot point

specifications will supersede or supplement the model's regular initial conditions.

AdH material properties are divided into two sets: global (e.g., gravity, **MP G**) and material-specific (e.g., hydraulic conductivity, **MP K**). Pilot point groups may describe a subset of groundwater and heat problem material specific properties that are suitable for spatial interpolation with the **PP MP** card, including the following:

- maximum refinement level
- refinement tolerance
- hydraulic conductivity
- porosity
- specific storage
- dispersivity
- tortuosity
- molecular diffusion
- retardation coefficient.

The pilot point group specification is confined to the given material's region(s) in the domain; the new property is interpolated at the centroid of each element assigned the material. Examples of an unsuitable material property are the water retention curves (pressure-relative conductivity and pressure-saturation) since X-Y series are necessary to describe these relationships, even if van Genuchten parameters are used. The majority of the permitted material properties are single real-data-type values representing characteristics that in reality are spatially heterogeneous and therefore are a perfect fit for pilot point specification; the following two cases are not as direct.

The key ability of AdH, the adaption of the mesh, is controlled by tolerances and level flags. Mesh elements are split, or refined, when the calculated error indicators at the elements are greater than a given refinement tolerance (e.g., **MP FRT**), and the elements' refinement levels are less than the given maximum (**MP ML**) where the *level* of an element is the number of times an element has been refined. A maximum refinement level of zero eliminates adaption. Mesh elements are merged, or unrefined, when the calculated error indicators are significantly smaller than the refinement tolerance. Pilot point specification may be utilized to control mesh adaption within a material region by spatially varying a

specific problem tolerance and/or the maximum level. The maximum level parameter is a discrete quantity; hence, the pilot point scheme's interpolated value (a real data type) is rounded up or down to the nearest integral value prior to its substitution.

The standard hydraulic conductivity card, **MP K**, requires six real-data-type values to describe the second-order symmetric tensor ($K_{XY} = K_{YX}$, $K_{XZ} = K_{ZX}$, and $K_{YZ} = K_{ZY}$). Tensor interpolation is not supported by AdH's pilot point specification, so three alternatives are provided to specify heterogeneity. Option 1: the originally specified hydraulic conductivity tensor may be scaled by a spatially varying factor. All tensor components are multiplied by the same factor. Option 2: the tensor may be superseded by two separate spatially varying horizontal and vertical conductivities ($K_H$ and $K_V$, respectively) where their respective off-diagonal tensor components are defaulted to zero. If $K_H$ is given, then $K_{XX} = K_{YY} = K_H$ and $K_{XY} = K_{YX} = K_{XZ} = K_{ZX} = K_{YZ} = K_{ZY} = 0$, while $K_{ZZ}$ is unchanged as shown in Figure 7. If $K_V$ is given, then $K_{ZZ} = K_V$ and $K_{XZ} = K_{ZX} = K_{YZ} = K_{ZY} = 0$ with the remaining components unchanged. Option 3: the tensor may be superseded at the individual component level ($K_{XX}$, $K_{XY}$, $K_{XZ}$, $K_{YY}$, $K_{YZ}$, $K_{ZZ}$). Multiple pilot point groups will be necessary to completely specify a material's hydraulic conductivity tensor. These three options are mutually exclusive at the material level; for a given material, specifying a scaling factor, horizontal conductivity, and $K_{ZZ}$ component are prohibited, but material 1 may specify a scaling factor; material 2, horizontal conductivity; and material 3, an individual component. It is not required that both $K_H$ and $K_V$, and, similarly, all the individual components, are specified. The original hydraulic conductivity may be partially superseded by pilot point specification.

The association parameter cards are mutually exclusive with one required for each pilot point group (Table 4).

#### *3.1.2.2 Group Properties*

These cards define the basic information of a pilot point group (a set of points with values representative of a given parameter) and the method to interpolate parameter values to the domain.

Pilot point specification may utilize a set of either 2D or 3D point locations, given by the **PP PT2** or **PP PT3** cards, respectively, though the available interpolation methods are limited for the lower dimension. In either case (2D or 3D), a list of labels, coordinates, and parameter values is required.

Figure 7. Hydraulic conductivity, K, tensor: (A) original; altered by option 1 (B) scale factoring (in red, bold); by option 2 (C) horizontal conductivity and (D) vertical conductivity; and by option3 individual components (E) $K_{XX}$ (red), $K_{YY}$ (green), $K_{ZZ}$ (blue), (F) $K_{XY}$ (red), $K_{XZ}$ (green), and $K_{YZ}$ (blue).

A)

$$K = \begin{bmatrix} K_{XX} & K_{XY} & K_{XZ} \\ K_{YX} & K_{YY} & K_{YZ} \\ K_{ZX} & K_{ZY} & K_{ZZ} \end{bmatrix}$$

D)

$$K = \begin{bmatrix} K_{XX} & K_{XY} & 0 \\ K_{YX} & K_{YY} & 0 \\ 0 & 0 & \boldsymbol{K_V} \end{bmatrix}$$

B)

$$\boldsymbol{S}K = \begin{bmatrix} \boldsymbol{S}K_{XX} & \boldsymbol{S}K_{XY} & \boldsymbol{S}K_{XZ} \\ \boldsymbol{S}K_{YX} & \boldsymbol{S}K_{YY} & \boldsymbol{S}K_{YZ} \\ \boldsymbol{S}K_{ZX} & \boldsymbol{S}K_{ZY} & \boldsymbol{S}K_{ZZ} \end{bmatrix}$$

E)

$$K = \begin{bmatrix} \boldsymbol{K_{XX}} & K_{XY} & K_{XZ} \\ K_{YX} & \boldsymbol{K_{YY}} & K_{YZ} \\ K_{ZX} & K_{ZY} & \boldsymbol{K_{ZZ}} \end{bmatrix}$$

C)

$$K = \begin{bmatrix} \boldsymbol{K_H} & 0 & 0 \\ 0 & \boldsymbol{K_H} & 0 \\ 0 & 0 & K_{ZZ} \end{bmatrix}$$

F)

$$K = \begin{bmatrix} K_{XX} & \boldsymbol{K_{XY}} & \boldsymbol{K_{XZ}} \\ \boldsymbol{K_{YX}} & K_{YY} & \boldsymbol{K_{YZ}} \\ \boldsymbol{K_{ZX}} & \boldsymbol{K_{ZY}} & K_{ZZ} \end{bmatrix}$$

Table 4. Association Parameter Cards

| PP HOT | INITIAL CONDITION PARAMETER | | |
|---|---|---|---|
| The PP HOT card specifies the initial domain condition a pilot point group represents for hot starting the simulation. The last field is conditional on the penultimate field. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | HOT | Parameter |
| 3 | string | “” | Initial condition:<br>IPH Pressure head (GW)<br>ITH Total head (GW)<br>IC Constituent (GW)<br>IT Temperature (Heat) |
| If initial condition is constituent (field 3 is equal to IC): | | | |
| 4 | int | ≥ 0 | Constituent ID |
| PP MP | MATERIAL PARAMETER | | |
| The PP MP card specifies the material property a pilot point group represents. The last field is conditional on a preceding field. It is noted that material IDs within AdH are no longer restricted to a consecutive series beginning with 1 but can be any integer value except the C language macro constant INT_MAX value (found in limits.h; actual value depends on operating system and library implemention). | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | MP | Parameter |

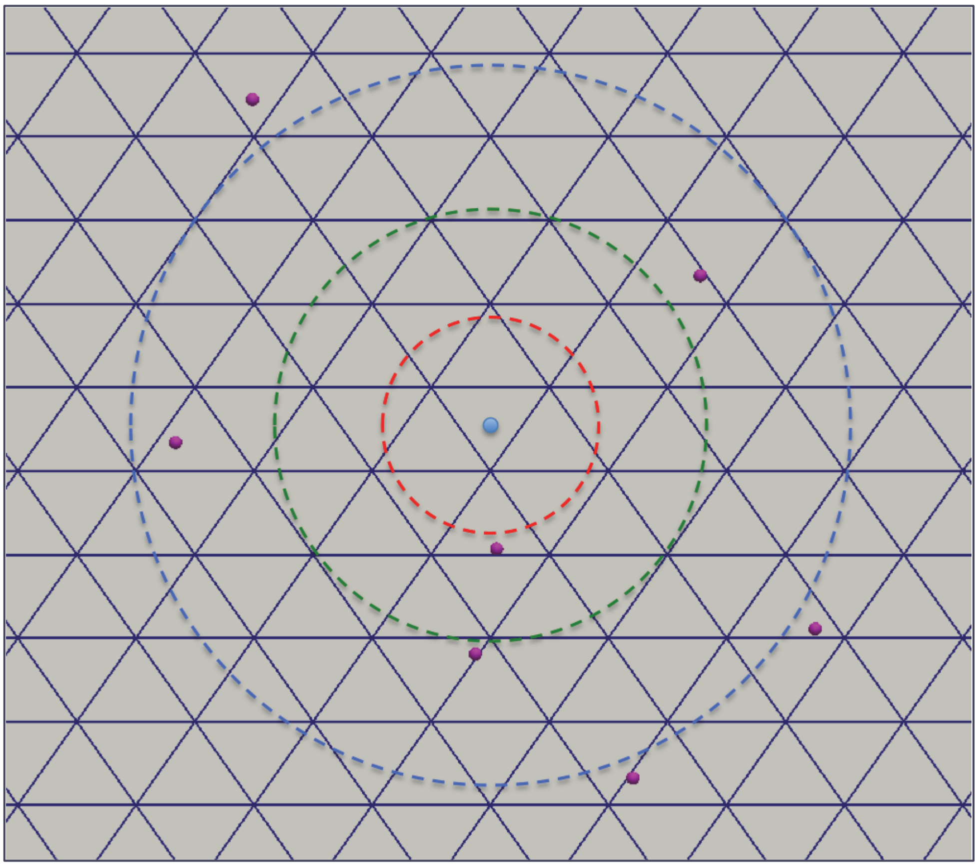
| | | | |
|---|---|---|---|
| 3 | string | “” | Material property:<br>DF Molecular diffusion (GW)<br>DPL Longitudinal dispersivity (GW & Heat)<br>DPT Transverse dispersivity (GW & Heat)<br>FRT Flow refinement tolerance (GW)<br>HRT Heat refinement tolerance (Heat)<br>KS Hydraulic conductivity scaling factor (GW)<br>KH Horizontal hyd. cond. (GW)<br>KV Vertical hyd. cond. (GW)<br>KXX Hyd. cond. tensor XX component (GW)<br>KXY Hyd. cond. tensor XY comp. (GW)<br>KXZ Hyd. cond. tensor XZ comp. (GW)<br>KYY Hyd. cond. tensor YY comp. (GW)<br>KYZ Hyd. cond. tensor YZ comp. (GW)<br>KZZ Hyd. cond. tensor ZZ comp. (GW)<br>ML Max. level of refinement (GW & Heat)<br>POR Porosity (GW and Heat)<br>RD Retardation (GW)<br>SS Specific storage (GW)<br>TOR Tortuosity (GW & Heat)<br>TRT Transport refinement tolerance (GW) |
| 4 | int | ≠ INT_MAX | Material ID |
| If material property is molecular diffusion, retardation, or transport refinement tolerance (field 3 is equal to DF, RD, or TRT, respectively): | | | |
| 5 | Int | ≥ 0 | Constituent ID |

The point labels are ignored by AdH but included to assist in the classification and visualization of points in other software. It is best practice to export point information from third-party applications such as Microsoft Excel or the Groundwater Modeling System (GMS).

The **PP RAD** card apportions the subset of pilot points involved in any given interpolation with a search radius and point count limits while the **PP LIM** card defaults or restricts the interpolated value. As shown in Figure 8, the search radius must be chosen wisely as it directly influences interpolation at the locations of interest. If the radius is too small, no pilot points may be found, and, therefore, interpolation cannot occur. Additionally, if the radius encircles fewer points than the given minimum requirement (e.g., specified minimum of 3 points, and the green circle in the Figure 8 is given), then interpolation will not occur. In the case of a large subset of pilot points where the count exceeds the given maximum limit, the points are prioritized by distance from the location of interest with the farthest points removed from the subset until the count is equal to the maximum count limit. AdH

does *not* include a method to sample pilot points by quadrant *nor* guarantees that the subset completely surrounds the location of interest. The distance between a pilot point and the location of interest is computed by Equations 1 and 2, based on the given interpolation scheme dimensionality.

Figure 8. Example pilot point search radii for locations of interest (blue point) that encircle zero, one, and four points (read, green, and blue dashed circles respectively).



3D:

$$d = \sqrt{\left(x_{loi} - x_{pt}\right)^2 + \left(y_{loi} - y_{pt}\right)^2 + \left(z_{loi} - z_{pt}\right)^2} \tag{1}$$

2D horizontal:

$$d = \sqrt{\left(x_{loi} - x_{pt}\right)^2 + \left(y_{loi} - y_{pt}\right)^2} \tag{2}$$

where:

$d$ = distance, L
$x_{loi}, y_{loi}, z_{loi}$ = coordinates of the location of interest, L
$x_{pt}, y_{pt}, z_{pt}$ = coordinates of the pilot point, L.

When search criteria are not satisfied and interpolation fails, the user-defined default is assigned at the location of interest. Two use cases must be acknowledged for this default value. First, specifying a blatantly invalid value can test a pilot point group's interpolation scheme and ensure complete coverage of the domain (or material region). The value may cause premature termination of AdH. Second, if desired spatial variance is limited, the default value can provide the standard parameter value to be augmented by interpolation. In other words, the default value can be either a flag for gaps or an intentional fill value.

After successful interpolation, the computed value is compared with given interpolation limits and restricted to the range as necessary. For example, given the desired range of 10 to 20, an interpolated value of 21 will be revised down to 20.

The interpolation method is declared using the **PP TYP** card and consists of two components: type and dimensionality. AdH currently provides three interpolation types that do *not* depend on *a priori* relationships of data points (e.g., Delaunay triangulation or Voronoi diagram):

- nearest-neighbor
- modified Shepard's method inverse-distance weighted (IDW)
- ordinary kriging

and two aforementioned dimensionalities:

- 3D
- 2D horizontal

for a combinatorial total of six schemes. The dimensionality component restricts which coordinates are used during computation, specifically in regard to distances. Three-dimensionality allows all coordinates to be included; 2D horizontal dimensionality ignores all *z*-coordinate (elevation) values by defaulting them to zero prior to computations. The 2D horizontal option was included for ease of use and allows simplifying assumptions, but it is inappropriate for vertically heterogeneous datasets of columnar points,

such as borehole samples. If a 3D interpolation method is specified, then full 3D pilot points must be also specified via **PP PT3**. The 3D interpolation methods (e.g., 3D ordinary kriging) require the use of **PP PT3**.

The simplest of AdH's interpolation types, nearest-neighbor, generates a piecewise-constant field of values by assigning the value of the closest pilot point. The minimum and maximum number of pilot points (**PP RAD**) must be equal to one for proper specification (enforced to avoid any confusion). Although not a smooth interpolant, this method is quick and may be used to make direct substitution of values. If the pilot point group contains a single point, and the search radius is greater than the domain extent's diagonal measure (i.e., the search radius envelopes the entire domain), the value is automatically stored in the normal material property data structure instead of being interpolated and stored at every element.

Inverse-distance weighting, one of the simplest linear interpolation methods, gives more significance to the closer pilot points and less to the more distant by using the distance between the pilot points and the location of interest. AdH modifies Shepard's classical formulation by setting the arbitrary weighting exponent to 2.0 and including the partial sample R-sphere mentioned by Franke and Nielson (1980), presented here as Equations 3 through 5.

Modified Shepard's method IDW:

$$\hat{v}(x_{loi}) = \sum_{i=1}^{n} w_i(x_{loi}) v(x_i) \tag{3}$$

$$w_i(x_{loi}) = \frac{m_i(x_{loi})}{\sum_{j=1}^{n} m_j(x_{loi})} \tag{4}$$

$$m_k(x_{loi}) = \left( \frac{R - d(x_{loi}, x_k)}{R * d(x_{loi}, x_k)} \right)^2 \tag{5}$$

where:

$\hat{v}$ = IDW estimator
$x_{loi}$ = location of interest
$w_i$ = IDW weight

$v$ = observed value
$x_i$ = pilot point
$m_i, m_j$ = modified weight
$R$ = R-sphere radius of influence
$d(x_{loi}, x_k)$= distance between location of interest and pilot point.

The R-sphere radius is set to the distance of the farthest pilot point in the subset to remove scaling effects from the computation. The downfall of the IDW interpolant is that it produces a distribution with local extrema at the pilot points and values trending towards the mean between the observations, which may not necessarily reproduce the understood distribution.

Kriging is a set of geostatistical methods to estimate unknown values based on variances between known observations (Equations 6-13). Ordinary kriging is the most common type of kriging as it is referred to as the "best linear unbiased estimator." "Best" is implied here "only in the least-squares error sense" (Deutsch and Journel 1998) for minimizing the error variance, $\sigma_R^2$. "Ordinary kriging is 'linear' because its estimates are weighted linear combinations of the available data; it is 'unbiased' since it tries to have $m_R$, the mean residual or error, equal to 0" (Isaaks and Srivastava 1989). This allows ordinary kriging to assume an unknown and constant mean as opposed to simple kriging where the mean must be specified, which is difficult with data collected in the field.

Kriging general equations:

$$\hat{v}(x_{loi}) = \sum_{i=1}^{n} w_i(x_{loi}) v(x_i) \tag{6}$$

$$m_R = \frac{1}{n}\sum_{i=1}^{n} R_i = \frac{1}{n}\sum_{i=1}^{n} \hat{v}_i - v_i \tag{7}$$

$$\sigma_R^2 = \frac{1}{n}\sum_{i=1}^{n} (R_i - m_R)^2 \tag{8}$$

where:

$\hat{v}$ = kriging estimator
$x_{loi}$ = location of interest

$w_i$ = kriging weight
$v$ = observed value
$x_i$ = pilot point location
$m_R$ = mean error
$R_i$ = error $(\hat{v}_i - v_i)$
$\sigma_R^2$ = error variance.

Ordinary kriging conditions:

$$m_R = 0 \tag{9}$$

$$\sum_{i=1}^{n} w_i = 1 \tag{10}$$

Ordinary kriging minimized error variance:

$$\sigma_R^2 = \sigma^2 - \left(\sum_{i=1}^{n} w_i C_{i,loi} + \mu\right) = \sigma^2 - \mathrm{w} \cdot \mathrm{D} \tag{11}$$

where:

$\sigma^2$ = variance
$C_{i,loi}$ = covariance of pilot point and location of interest
$\mu$ = Lagrange parameter
$w$ = weights vector
$D$ = covariance matrix (pilot point and location of interest).

Ordinary kriging system of equations:

$$C \cdot w = D \tag{12}$$

$$\begin{bmatrix} C_{1,1} & \cdots & C_{1,n} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ C_{n,1} & \cdots & C_{n,n} & 1 \\ 1 & \cdots & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} w_1 \\ \vdots \\ w_n \\ \mu \end{bmatrix} = \begin{bmatrix} C_{1,loi} \\ \vdots \\ C_{n,loi} \\ 1 \end{bmatrix} \tag{13}$$

where:

$C$ = covariance matrix (pilot points)
$C_{i,j}$ = covariance of pilot points.

Ordinary kriging currently is AdH's most computationally expensive interpolation scheme, but its flexibility creates the most customizable distribution with sparse data. To estimate a value, the covariances between individual pilot point locations and the location of interest are computed. These inform the linear system which is solved for the weights. Finally, the influential portions of the observed data, based on the weights, are summed. Additional information is required to compute the covariances used in the system of equations (see the Kriging Interpolation Properties section). For detailed discussion on ordinary kriging, see Chapter 12 of Isaaks and Srivastava (1989). AdH's kriging methods are based, in part, on the Geostatistical Software Library (GSLIB) (Deutsch and Journel 1998).

When 3D pilot points (**PP PT3**) are provided, it is fairly easy to switch among all six interpolation methods, compare the interpolants, and estimate the model sensitivity to the interpolation scheme.

The group property cards (Table 5), are required with **PP PT2** or **PP PT3** (mutually exclusive) for each pilot point group.

#### *3.1.2.3 Kriging Interpolation Properties*

These cards define the information specific to the kriging interpolation scheme and are necessary only if the **PP TYP** card specifies the ordinary kriging interpolation type. As mentioned in the general interpolation discussion above, the kriging interpolant estimates values influenced by covariances that are in turn derived from a semivariogram model. A semivariogram, or, simply, variogram, is a description of spatial variability as a function of distance, $\gamma(h)$. It is normally presented as a 1D scatter plot of observed data with a best-fit curve. For purposes in AdH, a variogram must be viewed as a 3D volume or at least a 2D surface description to handle anisotropy.

The key parameters of a variogram are as follows:

- nugget – the variance value at $h = 0$, technically should be equal to zero though sampling at very small distances may cause the variance to be nonzero; global background variance
- range – the distance at which the change in variance is negligible (where the variogram plateaus)
- sill – the variance value at the range; the maximum variance

- bearing angle – the direction of the major axis defined by the three components, measured in degrees:
  - azimuth – rotation around the $z$-axis from the $y$-axis (similar to yaw in aeronautics) where clockwise is positive
  - dip – rotation around the $x$-axis from the $z$-axis (pitch) where counterclockwise is positive
  - plunge – rotation around the $y$-axis from the $x$-axis (roll), where clockwise is positive
- anisotropy ratio – the relationship between the major axis and two orthogonal minor axes:
  - horizontal – the non-rotated $y$-axis and $x$-axis
  - vertical – the non-rotated $z$-axis and $y$-axis.

Table 5. Group Property Cards

| PP LIM | INTERPOLATION LIMITS | | |
|---|---|---|---|
| The PP LIM card is used to specify the interpolation limits for a pilot point group. The interpolated value is set to the respective limit if outside the given valid range. If interpolation cannot be performed (e.g., search criteria are not met), then the default value is used. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | LIM | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | int | # | Lower interpolation limit |
| 5 | int | # | Upper interpolation limit |
| 6 | int | # | Default interpolation value |
| PP PT2 | 2D PILOT POINTS | | |
| The PP PT2 card is used to specify a group of 2D pilot points, each with a location and parameter value. The number of lines is variable. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | PT2 | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | int | ≥ 1 | Number of points |
| An additional line with the following fields is expected for each point. Blank lines or comment lines, demarcated with a preceding # or !, may be interspersed, but the total number of point information lines must be provided prior to any other card. | | | |
| Secondary line (for each point) | | | |

| Field | Type | Value | Description |
|---|---|---|---|
| 1 | string | “” | Label (use single or double quotes for multiple words) |
| 2 | real | # | *X*-coordinate |
| 3 | real | # | *Y*-coordinate |
| 4 | real | # | Value |

| PP PT3 | 3D PILOT POINTS |
|---|---|

The PP PT3 card is used to specify a group of 3D pilot points, each with a location and parameter value. The number of lines is variable.

| Field | Type | Value | Description |
|---|---|---|---|
| 1 | string | PP | Card type |
| 2 | string | PT3 | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | int | ≥ 1 | Number of points |

An additional line with the following fields is expected for each point. Blank lines or comment lines, demarcated with a preceding # or *!*, may be interspersed, but the total number of point information lines must be provided prior to any other card.

Secondary line (for each point)

| Field | Type | Value | Description |
|---|---|---|---|
| 1 | string | “” | Label (use single or double quotes for multiple words) |
| 2 | real | # | *X*-coordinate |
| 3 | real | # | *Y*-coordinate |
| 4 | real | # | *Z*-coordinate |
| 5 | real | # | Value |

| PP RAD | SEARCH RADIUS |
|---|---|

The PP RAD card is used to specify the interpolation search parameters for a pilot point group. These parameters define the subset of points involved in the interpolation at a given domain location. If more points than the maximum (*m*) are found within the search perimeter, then only the closest *m* points are involved.

| Field | Type | Value | Description |
|---|---|---|---|
| 1 | string | PP | Card type |
| 2 | string | RAD | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | real | > 0 | Search Radius |
| 5 | int | ≥ 1 | Minimum number of points |
| 6 | int | ≥ minimum | Maximum number of points |

| PP TYP | INTERPOLATION METHOD |
|---|---|

The PP TYP card is used to specify the interpolation method for a pilot point group.

| Field | Type | Value | Description |
|---|---|---|---|
| 1 | string | PP | Card type |
| 2 | string | TYP | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | enum | ≥ 0 | Interpolation type:<br>0 Nearest-neighbor<br>1 Ordinary kriging<br>11 Modified Shepard's method inverse-distance weighted (IDW) |
| 5 | enum | ≥ 0 | Interpolation dimensionality:<br>0 3D<br>1 2D horizontal |

An omnidirectional variogram, defined by anisotropy ratios of one, depicts the same variance in any direction from a point. In this case the specified bearing angle is inconsequential. When the ratios are non-uniform, the bearing angle and the ratios determine a transformation matrix that scales and rotates the variogram to compute the proper $\gamma(h)$. It may be easier to understand the parameters of an anisotropic variogram as those necessary to transform a sphere into an ellipsoid with semi-major and semi-minor axes equal to the range. This imaginary ellipsoid would contain the volume within which the variability is increasing.

A sample variogram is usually derived during the analysis of observed data showing the relationship between known points. For kriging purposes, a variogram is necessary to describe the relationship between observed data and an unobserved location in the determination of weights where the "variogram distance measures the average degree of dissimilarity between an unsampled value $z(u)$ and a nearby data value. For example, given only two data values $z(u+h)$ and $z(u+h')$ at two different locations, the more *dissimilar* sample value should receive lesser weight in the estimation of $z(u)$" (Deutsch and Journel 1998). Used in this fashion, the variogram is referred to as a variogram model.

A variogram model is specified using a best-fit equation to express the change of variance between the nugget and sill. For complex descriptions, multiple expressions can be summed, referred to as nested variograms. The available variogram types are presented in Equations 14 through 20.

Nugget-effect:

$$\gamma(h)=\begin{cases}0, if\ h=0\\ c, if\ h>0\end{cases} \tag{14}$$

Spherical:

$$\gamma(h)=\begin{cases}c*\left[1.5\dfrac{h}{a}-0.5\left(\dfrac{h}{a}\right)^{3}\right], if\ h\leq 0\\ c, if\ h\geq 0\end{cases} \tag{15}$$

Exponential:

$$\gamma(h)=c*\left[1-exp\left(-\frac{3h}{a}\right)\right] \tag{16}$$

Gaussian:

$$\gamma(h)=c*\left[1-exp\left(-\frac{(3h)^{2}}{a^{2}}\right)\right] \tag{17}$$

Power:

$$\gamma(h)=c*h^{\omega} \tag{18}$$

Hole effect:

$$\gamma(h)=c*\left[1-\cos\left(\frac{h}{a}\pi\right)\right] \tag{19}$$

Dampened hole effect:

$$\gamma(h)=c*\left[1-exp\left(-\frac{3h}{d}\right)-\cos\left(\frac{h}{a}\pi\right)\right] \tag{20}$$

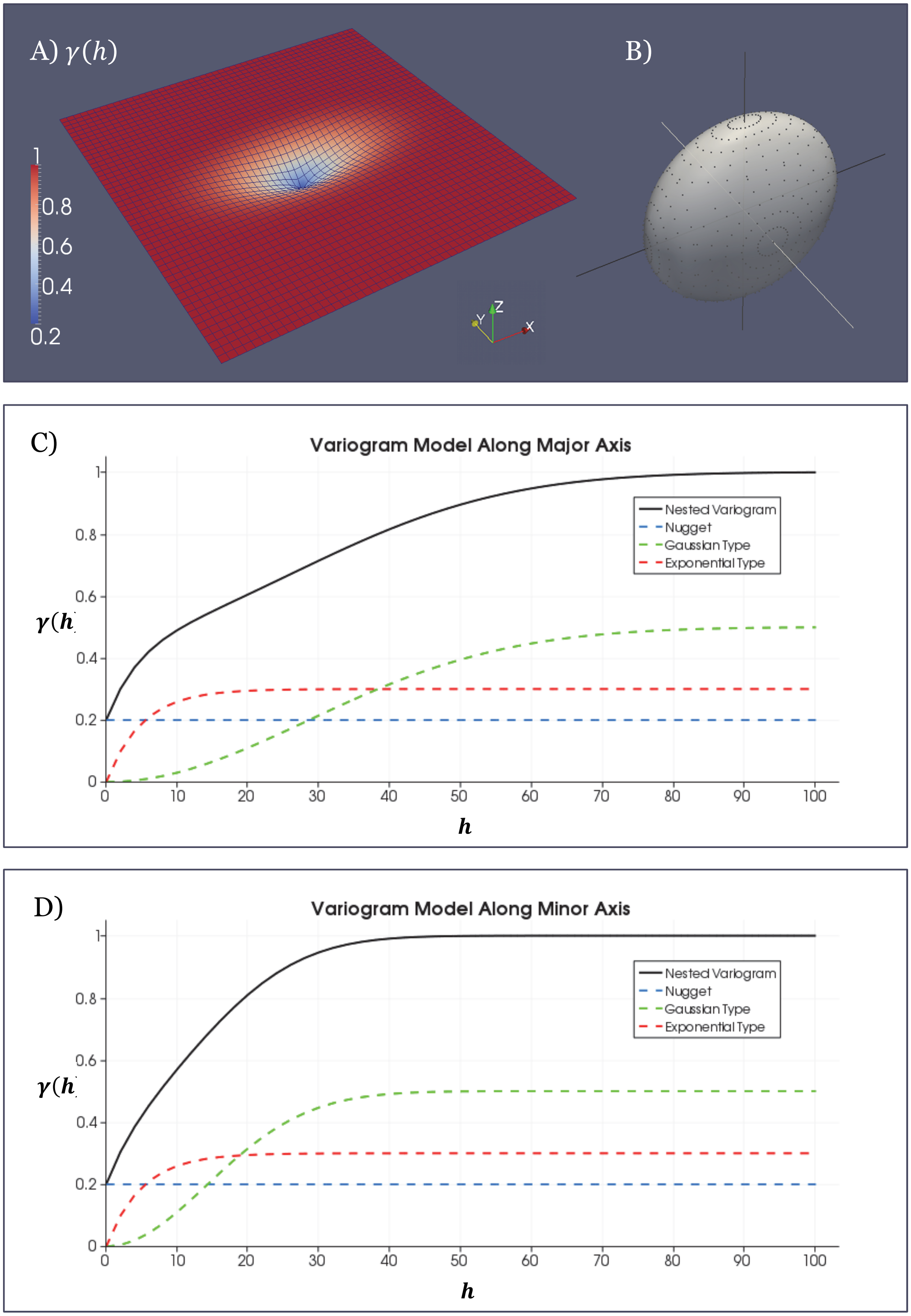
where:

$\gamma(h)$ = variogram variance
$h$ = variogram distance
$c$ = contribution
$a$ = range
$\omega$ = power exponent, $0 < \omega < 2$
$d$ = distance where 95% of the hole effect is dampened out.

The contribution ($c$) of the variogram type is the same concept as the sill; however, the term *sill* is reserved here for only the variogram model. The sill of a variogram model is equal to the sum of the nugget and all contributions. For variogram types that approach their contributions asymptotically (exponential and Gaussian), the range is the distance at which $\gamma(a) = 0.95c$. The power variogram type does not technically have a sill (i.e., it does not plateau), so the contribution is an arbitrary maximum value. An anisotropic, nested variogram model is shown in Figure 9. The model consists of a nugget of 0.2; an exponential type variogram with a contribution of 0.3 and range of 15; and a Gaussian-type variogram with a contribution of 0.5, major axis range of 70, horizontal anisotropy ratio of 0.5, and azimuth bearing angle of 90 degrees. The major axis is aligned with the *x*-axis.

To provide easy and flexible specification of variogram models, parameters are organized on multiple cards. An individual variogram's specific parameters are given on the **PP VG2** or **PP VG3** cards. The difference between the two versions is the user's approach in specifying parameters; use of **PP VG2** assumes that vertical transformation and rotations are unnecessary, and AdH defaults them appropriately. The **PP VG3** card requires the specification of all three bearing angles and both anisotropy ratios. The dimensionality of the variogram input does not limit the dimensionality of associated kriging interpolation. Either version provides the information necessary to construct a variogram to describe spatial variance in any 3D direction. The first characteristic of the variogram model, the number of variograms composing the model, is given on the **PP KRG** card. Since this number is variable, **PP VGI** lists the IDs of the variograms, thereby linking the pilot point group to **PP VG2** and **PP VG3** cards. Second, the variogram model nugget is given on **PP KRG** which is combined with the third characteristic, the individual variogram's contributions, listed on the **PP VGC** card, to produce the variogram model sill. The contributions must be listed in the same order as **PP VGI**.

Figure 9. Example variogram model shown as a surface (A) with the transformation matrix as an ellipsoid (B) and as traditional variogram plots along the principle axes (C & D).



In practice, the variance magnitude is not as important as the shape of the variogram. Therefore, the sill of a variogram model is often equal to one, $\gamma(a) = 1$, for the sake of simplicity. The **PP VGW** card is provided as an alternative to (and mutually exclusive with) **PP VGC** for those inclined to this concept. Instead of providing contributions, **PP VGW** lists the weights of the variograms in a similar fashion. With an assumed sill and a given nugget, the weights are used to divide the remainder and compute contributions for the user as defined by Equations 21 and 22.

Variogram contributions from weights:

$$c_i = \beta_i * \left[\gamma(a) - \gamma(0)\right] \tag{21}$$

$$\sum_{i=1}^{n} \beta_i = 1 \tag{22}$$

where:

$c_i$ = variogram contribution
$\beta_i$ = variogram weight
$\gamma(a)$ = variogram model sill
$\gamma(0)$ = variogram model nugget.

The weights are decimal fractions that must sum to 1.0 (100%). Due to the shape of the expression, **PP VGW** cannot be specified when including a power-type variogram. If necessary, the sill assumption can be overridden with the **PP VGS** card. This card may be given only when computing contributions from weights.

As stipulated by Isaaks and Srivastava (1998), "[i]f the major features of the sample variogram can be captured by a simple model, then it will provide solutions that are as accurate as those found using a more complex model. The principle of parsimony is a good guide in variogram modeling." For detailed discussion on modeling variograms see Chapters 16 and II.3 of Isaaks and Srivastava (1989) and Deutsch and Journel (1998), respectively.

The variogram model is converted to a covariance function for the purpose of kriging by the following relationship, Equation 23, based on the assumption that the random variables of ordinary kriging all have the same variance and mean.

Ordinary kriging variogram/covariance relationship:

$$C_{i,j} = \sigma^2 - \gamma_{i,j} \tag{23}$$

where:

$C_{i,j}$ = covariance
$\sigma^2$ = kriging variance
$\gamma_{i,j}$ = variogram model.

Finally, the kriging properties also include an option on the **PP KRG** card to utilize a log transformation in the interpolation. This may provide better results when interpolating a parameter from a sample with a range of multiple orders of magnitudes (e.g., hydraulic conductivity). When selected, the general equation, Equation 6, is replaced with Equation 24.

Kriging equation with log transformation:

$$\hat{v}(x_{loi}) = 10^{\left[\sum_{i=1}^{n} w_i(x_{loi}) \log_{10}(v(x_i))\right]} \tag{24}$$

where:

$\hat{v}$ = kriging estimator
$x_{loi}$ = location of interest
$w_i$ = kriging weight
$v$ = observed value
$x_i$ = pilot point location.

A set of kriging interpolation property cards (Table 6) is required for each pilot point group that specifies kriging interpolation. The number of variogram cards, however, does not necessarily correlate the number of kriging pilot point groups as variograms may be nested and/or shared by pilot point groups (referenced by multiple groups, therefore reusing the same spatial variability). **PP KRG** and **PP VGI** are required with one of the following combinations: **PP VGC**; **PP VGW**; or **PP VGW** and **PP VGS**. Variogram cards, **PP VG2** and **PP VG3**, are mutually exclusive with at least one required to perform kriging.

Table 6. Kriging Interpolation Property Cards

| PP KRG | KRIGING INFORMATION | | |
|---|---|---|---|
| The PP KRG card is used to specify the ordinary kriging interpolation parameters for a pilot point group. | | | |
| Field | Type | Value | Description |
| 1 | string | PP | Card type |
| 2 | string | KRG | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | real | ≥ 0 | Variogram model nugget |
| 5 | enum | ≥ 0 | Transform:<br>0 None<br>1 Log |
| 6 | int | ≥ 1 | Number of variograms |
| PP VGC | VARIOGRAM CONTRIBUTIONS | | |
| The PP VGC card is used to specify the contributions for variograms used in kriging interpolation for a pilot point group. The number of fields is variable. The number of variogram contributions (*n*) must match the number provided by the PP KRG card. The contributions reference the variograms listed by the PP VGI card (contributions are provided in the same order as the variogram IDs). | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | VGC | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | real | ≥ 0 | 1st variogram contribution |
| … | … | … | … |
| 3 + *n* | real | ≥ 0 | nth variogram contribution |
| PP VGI | VARIOGRAM IDS | | |
| The PP VGI card is used to specify which variograms are used for the kriging interpolation for a pilot point group. The number of fields is variable. The number of variogram IDs (*n*)must match the number provided by the PP KRG card. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | VGI | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | int | ≠ INT_MAX | 1st variogram ID |
| … | … | … | … |
| 3 + *n* | int | ≠ INT_MAX | nth variogram ID |

| PP VGS | VARIOGRAM SILL | | |
|---|---|---|---|
| The *optional* PP VGS is used to specify the sill of the variogram model used in kriging interpolation for a pilot point group when contributions are computed from variogram weights. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | VGS | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | real | ≥ 0 | Variogram model sill |

| PP VGW | VARIOGRAM WEIGHTS | | |
|---|---|---|---|
| The PP VGW card is used to specify the weights for variograms used in kriging interpolation for a pilot point group. The number of fields is variable. The number of variogram weights (*n*) must match the number provided by the PP KRG card. The weights reference the variograms listed by the PP VGI card (weights are provided in the same order as the variogram IDs). | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | VGW | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | real | ≥ 0 | $1^{st}$ variogram weight (decimal percent) |
| … | … | … | … |
| 3 + *n* | real | ≥ 0 | $n^{th}$ variogram weight (decimal percent) |

| PP VG2 | 2D VARIOGRAM INFORMATION | | |
|---|---|---|---|
| The PP VG2 card is used to specify a variogram with 2D parameters for use with kriging interpolation (vertical components are defaulted appropriately). The last fields are conditional on a preceding field. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | VG2 | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | enum | ≥ 0 | Variogram type:<br>0 Nugget-effect<br>1 Spherical<br>2 Exponential<br>3 Gaussian<br>4 Power<br>5 Hole effect<br>6 Dampened hole effect |
| 5 | real | ≥ 0 | Horizontal anisotropy ratio |
| 6 | real | \|#\| ≤ 360 | Azimuth bearing angle |
| If variogram type is power (field 4 is equal to 4): | | | |
| 7 | real | 0 < # < 2 | Variogram power exponent |

| | | | |
|---|---|---|---|
| Else: | | | |
| 7 | real | ≥ 0 | Major axis range |
| If variogram type is dampened hole effect (field 4 is equal to 6) | | | |
| 8 | real | > 0 | Variogram damping lag distance |
| PP VG3 | 3D VARIOGRAM INFORMATION | | |
| The PP VG3 card is used to specify a variogram with 3D parameters for use with kriging interpolation. The last fields are conditional on a preceding field. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | VG3 | Parameter |
| 3 | int | ≠ INT_MAX | Pilot point group ID |
| 4 | enum | ≥ 0 | Variogram type:<br>0 Nugget-effect<br>1 Spherical<br>2 Exponential<br>3 Gaussian<br>4 Power<br>5 Hole effect<br>6 Dampened hole effect |
| 5 | real | ≥ 0 | Horizontal anisotropy ratio |
| 6 | real | ≥ 0 | Vertical anisotropy ratio |
| 7 | real | \|#\| ≤ 360 | Azimuth bearing angle |
| 8 | real | \|#\| ≤ 360 | Dip bearing angle |
| 9 | real | \|#\| ≤ 360 | Plunge bearing angle |
| If variogram type is power (field 4 is equal to 4): | | | |
| 10 | real | 0 < # < 2 | Variogram power exponent |
| Else: | | | |
| 10 | real | ≥ 0 | Major axis range |
| If variogram type is dampened hole effect (field 4 is equal to 6) | | | |
| 11 | real | > 0 | Variogram damping lag distance |

#### *3.1.2.4 Miscellaneous*

The following **PP DBG** card, listed in Table 7, provides supplemental information regarding pilot point specification. It is unlikely to be used in general practice as its intent is to summarize input for testing purposes. For the sake of completeness, the card is included in this documentation.

Table 7. Miscellaneous Cards

| PP DBG | DEBUG INFORMATION | | |
|---|---|---|---|
| The presence of the *optional* PP DBG card causes AdH to print additional pilot point information with the regular screen output for review of input and to assist debugging. | | | |
| **Field** | **Type** | **Value** | **Description** |
| 1 | string | PP | Card type |
| 2 | string | DBG | Parameter |

## 3.2 Output

AdH will output the interpolated pilot point parameter values as datasets for inspection and verification in the eXentsible Data Model and Format (XDMF[1], maintained by Kitware, Inc.) file format that is viewable in the ParaView[2] visualization software (developed by Kitware, Inc.; Henderson 2007). The XDMF file format is a combination of XML *light* data and HDF5 *heavy* data so the raw data arrays can also be inspected with the HDFView[3] tool (developed by The HDF Group). Since mesh element data sets are not supported by the compatible ASCII file format, AdH cannot use the traditional output to provide pilot point data to the Department of Defense Groundwater Modeling System (GMS, developed by Aquaveo, LLC).

The resulting solution datasets of an AdH simulation (e.g., total head) are written as normal, incorporating the effects of the pilot point specification.

[1] http://www.xdmf.org/

[2] http://www.paraview.org/

[3] http://www.hdfgroup.org/HDF5/

# 4 Running AdH with Pilot Points

When all required input is ready, an AdH simulation utilizing pilot point specification is executed in the normal fashion with a pilot point-enabled version of the code. To verify the version of AdH executable, call the executable with the argument **-v** as shown with the resulting build information in Figure 10. The **PILOT_POINTS** keyword will be listed if enabled. Likewise, the inclusion of pilot point interpolated parameter fields in the output is dependent on the **XDMF** keyword.

Figure 10. Verifying AdH executable is pilot point enabled in a UNIX shell (Bash).

```
$ ./adh -v

 ---------------------
 AdH Build Information
 ---------------------
 SVN revision # 12324
 Build Date/Time: 2013.06.26 / 14:24:20
 Built with GW physics enabled
 Built with XDMF output file format
 Built with MPI enabled
 Built with PILOT_POINTS enabled
```

Although not necessary for regular groundwater problems, the pre-AdH executable may be run first to verify interpolated parameters. The difference between the pre-AdH and AdH executables is that the former does *not* proceed into the computational loops. Both executables read and verify the input, initialize the problem, perform pilot point interpolation, and write the interpolated parameters to the output. Pre-AdH may be verified and executed in a similar fashion to the full executable.

To run AdH, call the executable with the simulation base name as an argument (Figure 11). The executable build information is written to the screen, followed by runtime information, simulation input information, initialization, and, finally, the computational proceedings as shown in Figures 11 and 12. The former shows the head of the AdH output, while the latter shows the continuation of the output, though truncated, including the beginning of the computational loops. Check the runtime information section to ensure the proper simulation input files were provided to AdH. Either default or specified filenames will be listed, depending on whether an AdH super file is found. These are the files AdH will read to retrieve necessary input. Pilot point files will only be read if AdH is directed to include pilot point specification.

Figure 11. Running AdH executable in a UNIX shell (Bash).

```
$ ./adh Ex_sim

 ---------------------
 AdH Build Information
 ---------------------
 SVN revision # 12324
 Build Date/Time: 2013.06.26 / 14:24:20
 Built with GW physics enabled
 Built with XDMF output file format
 Built with MPI enabled
 Built with PILOT_POINTS enabled

 -------------------
 Runtime Information
 -------------------
 AdH execution Date/Time: 2013.05.23 / 14:30:37
 Launching AdH with project name: Ex_sim
 Launching AdH with run name: Ex_sim
 Found Super file named: Ex_sim.sup
 Default Geometry file name: Ex_sim.3dm
 Default Boundary condition file name: Ex_sim.bc
 Default Groundwater hotstart file name: Ex_sim.hot
 Specified Pilot Point file name: K-pts.txt (used if OP PP is specified)
 Specified Pilot Point file name: K-Kriged.txt (used if OP PP is specified)
 AdH was launched with 1 processor

 --------------------
 Geometry Information
 --------------------
 Number of 2D elements: 0
 Number of 3D elements: 54000
 Number of nodes: 10461
...
```

At runtime, AdH will read the pilot point files only after reading the standard input and finding the **OP PP** card. The **PP** cards are read and validated individually to confirm that card-level input criteria have been met. Then, each specified pilot point group is validated to ensure all specifications are complete and coherent. Any issues found during the validation routine will be listed in the Pilot Point Information section of the screen output (Figure 12) and cause AdH to terminate prematurely. Warnings regarding pilot point input, which do not require resolution, are also listed there. AdH attempts to validate all pilot point input in a single pass thus reducing the cycle of fixing one error only to find yet another during the subsequent model call. When all pilot point input is acceptable, a summary of the pilot point specification is provided in the Pilot Point Information section.

Next, AdH will link the pilot point groups to model parameters while assessing compatibility and uniqueness during the initialization routine. Compatibility includes pilot point group-to-pilot point group relationships (e.g., hydraulic conductivity components) and pilot point group-to-model relationships such as the existence of referenced materials and direct

Figure 12. Example AdH pilot point information screen output truncated with ellipses.

```
...
 ----------------------
 Pilot Point Information
 ----------------------
 Reading file: K-pts.txt

 Reading file: K-Kriged.txt

 Pilot point group 200:
 The kriging variogram model sill is assumed to be 1.0.

 Number of pilot point groups: 3
 Specified interpolated parameters:
 Type: Material property
 Material ID: 1 Parameter: Hydraulic conductivity scaling factor
 Material ID: 2 Parameter: Hydraulic conductivity scaling factor
 Material ID: 3 Parameter: Hydraulic conductivity scaling factor
 Specified interpolation methods:
 2D Horizontal Ordinary Kriging
 Total number of pilot points: 15
 Number of variograms: 3
...
 -------------------------
 Pilot Point Initialization
 -------------------------
 Initializing and linking pilot point data.
 Computing the point pair covariances for pilot point group 100.
 Computing the point pair covariances for pilot point group 200.
 Computing the point pair covariances for pilot point group 300.
 Interpolating the 3D elements' pilot point parameters.
 Completed pilot point data initialization.
...
 Printing solution at time: 0.00000e+00 0.00000e+00 Percent Done

 --------------------
 The Master Time Loop
 --------------------

 **************************************
 * Time Interval (0.000000, 1.000000) *
 **************************************
...
```

substitution with nearest-neighbor interpolation type. Once again, if any issues are found, they will be reported to the screen, this time in the Pilot Point Initialization section (Figure 12), and AdH will exit. Each pilot point group is interpolated to its respective domain entity at this time. Computed initial condition values are assigned directly to those mesh nodes without existing boundary condition assignments (which were already applied from standard input) for the initial solve. Interpolated material property values are stored in an auxiliary array structure that is linked to by the material data structure. If kriging is performed during the initial interpolation, the covariances between pilot point pairs are computed and also stored for future use.

Prior to the computational loop, AdH writes the model state of initial and boundary-condition forcings as the first solution output. The initial condition values based on pilot point specification are integrated into this first time-step of the data sets. All material property pilot point-based values are also written at this time as element field data with NaN (Not a

Number) reported at elements utilizing the standard zonal material property value.

As AdH sets up and solves the groundwater or heat transport problem, it normally retrieves material property parameters from the standard data structure. However, when pilot point specification is prescribed, AdH first checks whether a particular material property is linked to a spatially-varied data set and then retrieves the value from the auxiliary pilot point array structure or the standard data structure as necessary. As expected, this retrieval process taxes the simulation speed slightly, but the overall pilot point process was designed to balance speed with memory usage. Pilot point specification is integrated into AdH's domain decomposition for parallel processing and domain adaption routines. Every processor holds the pilot point specification input information, but the spatially-varying data held by the auxiliary array structure is limited to each processor's subdomain. When the mesh is refined or unrefined, the auxiliary array structure is updated to match the number of elements and new pilot point-based values are interpolated for each adapted element since their centroids changed. The new pilot point data is also written when the new mesh topology is outputted.

Given the values assigned through the pilot point process, AdH will operate and finish normally. Pilot point specification only substitutes values; the use of these values is not altered.

# References

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# Appendix: Pilot Point Input File Examples

## Example A

Simulation Ex_sim_A shows pilot point specification in default location and consists of the following files:

- Ex_sim_A.3dm – mesh geometry file
- Ex_sim_A.bc – boundary condition file (shown below)
- Ex_sim_A.hot – hotstart, or initial condition, file
- Ex_sim_A.pp – pilot point specification file (shown below)

***Ex_sim_A.bc*** (truncated with ellipses)

```
OP GW
OP PP # Enable pilot point specification
OP TRN 0
...
MP G 73231257600.0 # Gravity, m/day^2 (9.81 m/s^2)
MP RHO 1060.0 # Density, kg/m^3 (1.06e6 g/m^3)
MP MU 86.5728 # Viscosity, g/(m*s) (1.002 g/(m*s)

# Material 1 – Top Layer
MP K 1 3.0e-1 3.0e-1 3.0e-2 0.0 0.0 0.0 # Hydraulic conductivity, m/day
MP POR 1 0.4 # Porosity
MP SS 1 1.0e-5 # Specific storage, 1/m
...
```

***Ex_sim_A.pp***

```
# Material 1 Hydraulic conductivity scaling
PP MP KS 100 1 # parameter, pilot point group id, material id
PP TYP 100 11 1 # ppg id, interp type (IDW), interp dim (2D horiz)
PP RAD 100 120.0 2 5 # ppg id, search radius, min pts, max pts
PP LIM 100 0.1 10.0 -999 # ppg id, low bound, high bound, default value

PP PT2 100 5 # ppg id, num pts
SW 0.0 0.0 2.15 # pt label, X, Y, value
SE 90.0 0.0 3.37
Well 60.0 30.0 1.00
NE 90.0 60.0 0.92
NW 0.0 60.0 0.22
```

## Example B

Simulation Ex_sim_B shows pilot point specification in the ADH input file, referenced by the super file, and consists of the following files:

- Ex_sim_B.3dm – mesh geometry file
- Ex_sim_B.bc – boundary condition file (shown below)
- Ex_sim_B.hot – hotstart, or initial condition, file

- Ex_sim_B.sup – simulation super file (shown below)

***Ex_sim_B.bc*** (truncated with ellipses)

```
OP GW
OP PP # Enable pilot point specification
OP TRN 0
...
MP G 73231257600.0 # Gravity, m/day^2 (9.81 m/s^2)
MP RHO 1060.0 # Density, kg/m^3 (1.06e6 g/m^3)
MP MU 86.5728 # Viscosity, g/(m*s) (1.002 g/(m*s)

# Material 1 - Top Layer
MP K 1 3.0e-1 3.0e-1 3.0e-2 0.0 0.0 0.0 # Hydraulic conductivity, m/day
MP POR 1 0.4 # Porosity
MP SS 1 1.0e-5 # Specific storage, 1/m
...
# Material 1 Hydraulic conductivity scaling
PP MP KS 100 1 # parameter, pilot point group id, material id
PP TYP 100 11 1 # ppg id, interp type (IDW), interp dim (2D horiz)
PP RAD 100 120.0 2 5 # ppg id, search radius, min pts, max pts
PP LIM 100 0.1 10.0 -999 # ppg id, low bound, high bound, default value

PP PT2 100 5 # ppg id, num pts
SW 0.0 0.0 2.15 # pt label, X, Y, value
SE 90.0 0.0 3.37
Well 60.0 30.0 1.00
NE 90.0 60.0 0.92
NW 0.0 60.0 0.22
...
```

***Ex_sim_B.sup***

```
PP Ex_sim_B.bc
```

## Example C

Simulation Ex_sim_C shows pilot point specification in multiple files, referenced by the super file, and consists of the following files:

- Ex_sim_C.3dm – mesh geometry file
- Ex_sim_C.bc – boundary condition file (shown below)
- Ex_sim_C.hot – hotstart, or initial condition, file
- Ex_sim_C.sup – simulation super file (shown below)
- Mat1_K_IDW.txt – pilot point specification file (shown below)
- Mat1_K_pts.txt – pilot point specification file (shown below)

***Ex_sim_C.bc*** (truncated with ellipses)

```
OP GW
OP PP # Enable pilot point specification
OP TRN 0
...
MP G 73231257600.0 # Gravity, m/day^2 (9.81 m/s^2)
MP RHO 1060.0 # Density, kg/m^3 (1.06e6 g/m^3)
MP MU 86.5728 # Viscosity, g/(m*s) (1.002 g/(m*s)

# Material 1 – Top Layer
MP K 1 3.0e-1 3.0e-1 3.0e-2 0.0 0.0 0.0 # Hydraulic conductivity, m/day
MP POR 1 0.4 # Porosity
MP SS 1 1.0e-5 # Specific storage, 1/m
...
```

***Ex_sim_C.sup***

```
PP Mat1_K_pts.txt
PP Mat1_K_IDW.txt
```

***Mat1_K_IDW.txt***

```
# Material 1 Hydraulic conductivity scaling
PP MP KS 100 1 # parameter, pilot point group id, material id
PP TYP 100 11 1 # ppg id, interp type (IDW), interp dim (2D horiz)
PP RAD 100 120.0 2 5 # ppg id, search radius, min pts, max pts
PP LIM 100 0.1 10.0 -999 # ppg id, low bound, high bound, default value
```

***Mat1_K_pts.txt***

```
# Material 1 Hydraulic conductivity scaling
PP PT2 100 5 # ppg id, num pts
SW 0.0 0.0 2.15 # pt label, X, Y, value
SE 90.0 0.0 3.37
Well 60.0 30.0 1.00
NE 90.0 60.0 0.92
NW 0.0 60.0 0.22
```

## Example D

Simulation Ex_sim_D shows ordinary kriging interpolation method pilot point specification in the default location and consists of the following files:

- Ex_sim_D.3dm – mesh geometry file
- Ex_sim_D.bc – boundary condition file (shown below)
- Ex_sim_D.hot – hotstart, or initial condition, file
- Ex_sim_D.pp – pilot point specification file (shown below)

## ***Ex_sim_D.bc*** (truncated with ellipses)

```
OP GW
OP PP # Enable pilot point specification
OP TRN 0
...
MP G 73231257600.0 # Gravity, m/day^2 (9.81 m/s^2)
MP RHO 1060.0 # Density, kg/m^3 (1.06e6 g/m^3)
MP MU 86.5728 # Viscosity, g/(m*s) (1.002 g/(m*s)

# Material 1 – Top Layer
MP K 1 3.0e-1 3.0e-1 3.0e-2 0.0 0.0 0.0 # Hydraulic conductivity, m/day
MP POR 1 0.4 # Porosity
MP SS 1 1.0e-5 # Specific storage, 1/m
...
```

## ***Ex_sim_D.pp***

```
# Variograms
# variogram id, variogram type (gsn), horiz anisotropy, bearing angle, range
PP VG2 -100 3 1.0 0.0 15.0
PP VG2 -200 2 0.5 90.0 70.0

# Material 1 Hydraulic conductivity scaling
PP MP KS 100 1 # parameter, pilot point group id, material id
PP TYP 100 1 1 # ppg id, interp type (kriging), interp dim (2D horiz)
PP KRG 100 0.2 0 2 # ppg id, nugget, transform (log), num variograms
PP VGI 100 -100 -200 # ppg id, 1st variogram id, ...
PP VGC 100 0.3 0.5 # ppg id, 1st variogram contrib, ...
PP RAD 100 120.0 2 5 # ppg id, search radius, min pts, max pts
PP LIM 100 0.1 10.0 -999 # ppg id, low bound, high bound, default value

PP PT2 100 5 # ppg id, num pts
SW 0.0 0.0 2.15 # pt label, X, Y, value
SE 90.0 0.0 3.37
Well 60.0 30.0 1.00
NE 90.0 60.0 0.92
NW 0.0 60.0 0.22
```

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**14. ABSTRACT**
Guidelines are presented herein for using the US Army Corps of Engineers (USACE) Adaptive Hydraulics/Hydrology (AdH) modeling software to model three-dimensional groundwater problems with constituent or heat transport utilizing pilot point specification. Pilot point specification is an auxiliary module intended to be a flexible method to specify spatially varying parameters that supersede the traditional uniform parameters in the model. Examples of such parameters are hydraulic conductivity, porosity, and mesh refinement. Spatial variation can be used to develop high-fidelity computer models. This document contains descriptions of the pilot point input cards and examples.

The pilot point specification module is currently integrated into the AdH Groundwater code (kernel version), but can be extended to additional AdH physics modules as necessary. Input is currently manually generated with result viewable utilizing the open-source ParaView visualization software.

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